# Alignment of suprathermally rotating grains

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# ABSTRACT

It is shown, that mechanical alignment can be efficient for suprathermally rotating grains, provided that they drift with supersonic velocities. Such a drift should be widely spread due to both Alfvénic waves and ambipolar diffusion. Moreover, if suprathermal rotation is caused by grain interaction with a radiative flux, it is shown, that mechanical alignment may be present even in the absence of supersonic drift. This means that the range of applicability of mechanical alignment is wider that it is generally accepted and it can rival the paramagnetic one. We also study the latter mechanism and reexamine the interplay between poisoning of active sites and desorption of molecules blocking the access to the active sites of H<sub>2</sub> formation in order to explain the observed poor alignment of small grains and good alignment of large grains. To have a more comprehensive picture of alignment we briefly discuss the alignment by radiation fluxes and caused by grain magnetic moments.

**Key words:** magnetic fields – polarization – dust extinction.

#### INTRODUCTION

The polarimetry of the interstellar medium (hereafter ISM) testifies that dust grains are aligned. The original explanation of this phenomenon in Davis & Greenstein (1951) as being due to paramagnetic relaxation was later criticized in Jones & Spitzer (1967) as inadequate unless enhanced imaginary part of grain magnetic susceptibility was assumed. At the same time, alignment involving purely mechanical processes, pioneered in Gold (1951, 1952), was shown to have its own problems (see Davis 1955, Purcell 1969, Purcell & Spitzer 1971). A new important contribution to the field was done by Roberge & Hanany (1990), who proposed an interesting idea, that grain alignment can be caused by ambipolar diffusion. A comprehensive study of alignment of thermally rotating grains through the ambipolar diffusion is given in Roberge, Messinger, & Hanany (1995). Such an alignment is likely to be important for molecular clouds. However it is possible to show, that supersonic ambipolar diffusion cannot persist over extensive regions of the ISM.

A really profound step in elucidating the dynamics of the ISM dust grains was done by Purcell (1975, 1979) who introduced a concept of suprathermal rotation. However, it was shown in Spitzer & McGlynn (1979) that this only marginally improves the efficiency of paramagnetic alignment for high rates of resurfacing. In fact, specialists in the field believe that 'a relaxation mechanism orders of magnitude more efficient than that given by normal paramagnetism' is required (Chlewicki & Greenberg 1990).

This paper was preceded by our earlier papers devoted to the same issue. First, in Lazarian (1994) (henceforth Paper I) we provided a quantitative description of mechanical alignment of non-spherical grains. However, at that point it was unclear whether grains can be aligned mechanically, if they rotate at suprathermal velocities. Therefore, only alignment of thermally rotating grains was discussed. Then, in Lazarian (1995a) (henceforth Paper II) we addressed the problem of paramagnetic alignment of suprathermally rotating grains and showed that diffusion of oxygen over grain surface and existence of potential barrier for H<sub>2</sub> formation (Tielens & Allamandola 1987) bring into being the grain critical size  $l_{cr}$  and the critical number of active sites  $\nu_{cr}$ . It was found out that for grains with sizes less than  $l_{cr}$ suprathermal rotation due to H<sub>2</sub> formation is suppressed and that the poisoning of active sites is accelerated when the number of active sites becomes greater than  $\nu_{cr}$ . However, only the case  $\nu < \nu_{cr}$  was quantitatively discussed and no processes of desorption were invoked; this is a disadvantage of the latter study.

The aim of this paper is to determine roughly the relative importance of processes, that can provide alignment of suprathermally rotating grains. Therefore the contribution

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is rather miscellaneous. First of all, in Sect. 2 we remind our reader of the Purcell's concept of suprathermal rotation. Then, we address in Sect. 3 mechanical processes, which are usually believed to be incapable of aligning suprathermally rotating grains. We show that this is not true and discuss a process that can provide efficient alignment of such grains. In Sect. 4 we address the paramagnetic alignment and discuss poisoning of grain active sites when  $\nu > \nu_{cr}$  and the processes of desorption of molecules blocking the access to active sites. To provide a more comprehensive picture of alignment of suprathermally rotating grains, we touch upon the alignment of helical grains, grains subjected to radiative flows, as well as alignment due to grain magnetic moments.

#### 2 SUPRATHERMAL ROTATION OF GRAINS

Here we discuss the suprathermal rotation due to formation of  ${\rm H}_2$  molecules on the ISM grains. The number of molecules ejected per second from an individual site is  $\sim \gamma_1 l^2 n_H v_1 \nu^{-1}$ , where  $\gamma_1$  is the portion of H atoms absorbed by a grain of diameter l while  $\nu$  is the number of sites. A recoil from a molecule departing the grain is  $m_{H2}v_{H2}=(2m_{H2}E_{H2})^{1/2}$ , where  $E_{H2}$  is the kinetic energy of  ${\rm H}_2$  molecule (0.2 eV) (Williams 1988). Then the average squared z component of torque is

$$\langle [M_z]^2 \rangle \approx \frac{\gamma_1^2}{32} l^6 n_H^2 m_{H2} v_1^2 E_{H2} \nu^{-1}.$$
 (1)

Thus an individual grain spins up to high angular velocities, limited only by friction forces. As a result, the attainable value of angular velocity  $\Omega$  is proportional to  $\langle [M_z]^2 \rangle^{1/2} \kappa^{-1}$ , where  $\kappa$  is the constant of rotational friction  $\sim I_z t_d^{-1}$ . Note, that  $I_z$  is the z component of the momentum of inertia and  $t_d$  is the rotational dumping time. The latter is

$$t_d \approx Ct_m = C\frac{\varrho_s V}{S\Phi},$$
 (2)

where  $t_m$  is the time that takes a grain to collide with gaseous atoms of the net mass equal to the mass of the grain, V and  $\varrho_s$  are grain volume and density respectively; S is the grain cross-section for a supersonic flux, the coefficient C=0.6 is a precise result for a spherical grain (Purcell & Spitzer 1971) and  $\Phi$  is the mass flux which is  $v_1nm_a$  for supersonic  $v_1$ . Therefore assuming  $\gamma_1=0.2$  and  $n_H=n$ , one obtains  $\Omega\approx 2\cdot 10^8~{\rm s}^{-1}$ , for  $\nu=10^2$ .

Some grains are not subjected to the torques caused by  $\rm H_2$  formation. For instance, it was shown in Paper II that those are aromatic carbonaceous grains, as  $\rm H_2$  molecules are being formed is states of low excitation over their surface (Duley & Williams 1993). Nevertheless, such grains can rotate suprathermally, for instance, due to variations of the accommodation and/or photoelectric emission coefficients (see Purcell 1979). Further on, we will show that unlike suprathermal rotation due to  $\rm H_2$  formation, some of those processes may result in alignment on their own.

Our estimates of  $\Omega$  above are relevant to the long-lived spin-up (Spitzer & McGlynn 1979). For short-lived spin-up, namely, the correlation time of Purcell rockets  $t_L$  is much less than  $t_d$  our estimate of  $\Omega$  must be multiplied by  $\sqrt{t_L/t_d}$ . Speaking about Purcell alignment we will be mostly concerned with the long-lived spin-up. Paramagnetic

alignment corresponding to the short-lived spin-up does not differ much from the Davis-Greenstein one corresponding to the enhanced temperature of grain rotation  $KT_{qas}$ , where

$$K = \frac{I_z \langle [M_z]^2 \rangle t_d t_L}{k T_{gas}}.$$
 (3)

It was pointed out by Bruce Draine (private communication), that such an enhancement can be essential in molecular clouds where temperatures of gas and grains are very close.

In fact, suprathermal rotation can arise not only from  $\rm H_2$  formation, but also by the variations of the accomodation coefficient. We discuss these such processes in Section 5, as we show, that such variations can cause mechanical alignment of its own irrespectively from the action of the paramagnetic relaxation.

#### 3 MECHANICAL ALIGNMENT

#### 3.1 Supersonic motions

To produce mechanical alignment grains should drift supersonically in respect to gas. In Paper I it is showed that Alfvénic perturbations are efficient in providing supersonic drift perpendicular to magnetic field lines. Two main phenomena may be invoked: Alfvénic waves and ambipolar diffusion.

It is generally accepted, that supersonic drift by ambipolar diffusion is present within sufficiently strong shocks (see fig.1 in Pilipp et al 1990). However, this cannot be the cause of alignment for the majority of the ISM grains. Indeed, it was pointed out by B.Draine, that the dissipation due to ion-neutral streaming with velocity  $v_{in}$  is approximately

$$G = 0.5nn_i \langle \sigma_T v_T \rangle m_a v_{in}^2 \tag{4}$$

which for supersonic  $v_{in}=1 \,\mathrm{km\ s^{-1}}$  provides a dissipation rate per H atom  $G/n \approx 1.7 \times 10^{-25} \,\mathrm{erg\ s^{-1}}$ , which is well in excess of the energy that supernova is likely to eject into the turbulent motions. In other words, the ambipolar diffusion may be important for molecular clouds and localized regions in within diffuse clouds, but for the large scale alignment other processes must be invoked.

It was hinted in Paper I that large grains are inertial and therefore should decouple from ionized gas in the course of high frequency Alfvénic oscillations. Although this process of alignment does not entail strong dissipation, it is possible to show that the limitations imposed on grain size by both damping of high frequency Alfvénic waves and grain charge are rather strict.

Indeed, if a grain without electric charge is placed within partially ionized gas subjected to Alfvénic perturbations, e.g. with velocity  $v = v_0 \sin \omega_A t$ , it is easy to see that the amplitude of grain drift scales as  $v_0/\sqrt{1+\mu^2}$ , where  $\mu \approx 0.4(\rho_n/\rho_g)(v_0/(l\omega_A))$  and  $\rho_n$  and  $\rho_g$  are, respectively, gas and grain densities. Therefore  $\mu < 1$  provides the first constrain. In its turn, Alfvénic frequency cannot be arbitrary, as the waves of frequency higher than that of collisional frequency for ions are critically damped (see McKee et al 1994). The corresponding value of  $\omega_{cr}$  provides the minimal value of  $\mu$ . Another constrain stems from the grain

charge, as if  $\omega_A$  is less than the grain Larmour frequency, the drift velocity scales as  $v_0(\omega_A/\omega_L)$ . For a given grain size only oscillations within the range  $\omega_L < \omega_A < \omega_{cr}$  are efficient in the sense of providing supersonic drift. Therefore, even if the overall non-thermal line broadening of emission lines is observed, it is not clear a priori for a given grain, that this inequality is fulfilled and that the Alfvénic motions within aforementioned range of frequencies are supersonic. The estimates in Lazarian (1995b) show, that for the ionization ratio  $10^{-4}$  it is difficult to expect grains with radii less than  $10^{-5}$  cm to experience supersonic drift in the diffuse ISM, if grains are collisionally charged (see Spitzer 1978, Draine & Sutin 1987). It is gratifying, that such a dichotomy is observed and grains of sizes less than  $10^{-5}$  cm are not aligned (Kim & Martin 1994, 1995).

Radiation pressure can also cause grain drift. For this drift to be supersonic the following inequality  $Q_{ext}P_{rad}$  >  $4P_{gas}$  should be satisfied (Purcell 1969), where  $Q_{ext}$  is the ratio of the optical to geometrical cross sections, while  $P_{rad}$ and  $P_{qas}$  are, respectively, radiation and gaseous pressures. For hydrogen with density 10 cm<sup>-3</sup> and temperature 100 K,  $P_{gas} \approx 10^{-13} \ {
m dyn/cm^{-2}}$ . Usually  $Q_{ext} < 1$  and this means that it is difficult to obtain sufficient radiation pressure to account for large-scale ISM polarization. Thus supersonic drift due to radiation pressure is confined to regions in the vicinity of bright sources. As grains carry charge, their motion under the radiation pressure is usually constrained to following magnetic field lines (Spitzer 1978, p. 202). It is shown in Habing et al. (1994) that grains should move with supersonic relative velocities within the outflows around cool giants (carbon-stars, Mira variables and OH/IR stars) due to radiation pressure. The velocities of metallic grains should be greater than those of dielectric grains in such circumstances (Il'in 1994) and this may have observational consequences in view of mechanical alignment.

To summarize, supersonic drift is an essential feature of interstellar grain dynamics. In the vicinity of stars this drift takes place mostly due to radiation pressure and happens along magnetic field lines. Within molecular and atomic clouds at sufficient distances from bright sources, this drift takes place due to Alfvénic perturbations and grains move mostly perpendicular to magnetic field lines.

# 3.2 Cross section alignment

Grain alignment can be quantitatively described by the following measure:

$$\sigma_J = \frac{3}{2} \left\langle \cos^2 \beta - \frac{1}{3} \right\rangle,\tag{5}$$

where  $\beta$  is the angle between the angular momentum and the alignment axis. The latter can coincide with the direction of a corpuscular flux, if precession on the time scale of alignment is negligible, or with the direction of magnetic field, if the period of grain precession is much smaller than the said time scale. For suprathermally rotating grains the axis of major inertia is tightly coupled to the angular momentum (Purcell 1979). Therefore for oblate spheroidal grains,  $\sigma_J$  coincides with the Rayleigh reduction factor  $\sigma$  introduced in Greenberg (1968). For prolate spheroids it is easy to show that  $\sigma = -0.5\sigma_J$ .

One of the major questions that we need to answer here is whether suprathermally rotating grains can be aligned by a supersonic flow. A naive answer would be "no" as such rapidly rotating grains resemble gyroscopes and therefore should not be sensitive to gaseous bombardment. However, this answer ignores the role of crossovers. Further on we will show, that when both random and regular torques are dominated by recoils caused by H<sub>2</sub> formation, an efficient alignment of non-spherical grains is possible.

We remind our reader, that during crossovers grain angular velocity becomes close to zero and a substantial randomization of  $\bf J$  is present. A comprehensive theory of crossovers is given in Spitzer & McGlynn (1979) and further on we will use the results of this study.

Let us assume, for simplicity, that randomization is complete during a crossover, which is apparently true for sufficiently small grains (see Paper II for an explicit expression of the disorientation parameter). An incomplete randomization only alters the time of alignment. For instance, grain may need not one, but several crossovers to come to the state uncorrelated with an initial one. This, however, does not change anything for our further treatment.

If  $t_L$  is a characteristic correlation time for the existence of the sites of  $H_2$  formation, the mean time back to crossover is given by

$$t_x \approx 1.3(t_d + t_L) \tag{6}$$

(Purcell 1979). Usually, it is assumed that the time of the existence of active sites is the time necessary for accreting a monolayer of refractory material (Spitzer & McGlynn 1979). Another process that can determine  $t_L$  is poisoning of the active sites (see Paper II and Sect. 4 of this paper). However, for our simplified treatment we do not distinguish between the two processes limiting the life time of Purcell's rockets. Indeed, what is important for us is that, for a chosen grain,  $t_L$  is the time of accreting of N heavy atoms. The latter value depends on particular processes involved, but we will see that this is not critical for the mechanism below.

Consider at first a toy model, namely, assume that the axis of suprathermally rotating oblate grain can have only two positions, namely perpendicular  $(\bot)$  and parallel (||) to the axis of a gaseous flux. In this model, grain axis stays for the time  $t_x$  in one position and then undergoes the crossover and has equal chances to get either the same or the perpendicular alignment (disorientation is complete!). In the absence of the gaseous flux time scales  $t_{x\parallel}$  and  $t_{x\perp}$  are the same and, naturally, there is no preferential position. However, if the gaseous supersonic flux is present,  $t_d$  given by Eq. (2) is inversely proportional to gas-grain cross sections  $S_{n\parallel}$  and  $S_{n\perp}$  in the two positions. Moreover, it is natural to assume that the number of heavy atoms adsorbed by the grain is proportional to the overall number of atoms striking it. Thus  $t_L$  and  $t_x$  are both inversely proportional to the cross section. Assuming that the time of the crossover is negligible as compared with the time of a spin-up, we conclude that for an individual grain the time averaged probability of finding the grain in a position  $\perp$  or  $\parallel$  is inversely proportional, respectively, to  $S_{n\perp}$  and  $S_{n\parallel}$ . To find the constant of proportionality one needs to recall, that the probability of finding the grain in either of two positions is unity. According to the ergodic hypothesis this probability coincides with the ensemble averaged one.

The above considerations can be generalized. It is easy to see, that for a continues distribution of axis positions the probability of finding grain axis within at a particular angle is inversely proportional to the cross section corresponding to this angle.

It was assumed above, that both  $t_L$  and  $t_d$  are controlled by the same process, namely, by the interaction of a gaseous flow with a grain. One may imagine situations when  $t_L$  and  $t_d$  are controlled by different physical processes. If one of the times  $t_L$  or  $t_d$  is much less than the other,  $\dagger$  the longest of the two controls the alignment. For instance, for  $t_L \ll t_d$  we deal with alignment by friction, which may remind one the the idea suggested in Salpeter & Wickramssinghe (1969). However, these processes are different, as we deal here with suprathermally rotating grains, while Salpeter & Wickramasinghe discussed alignment of grains with enhanced rotational temperature. It is possible to show, that the alignment in the latter case is rather marginal. In the opposite limiting case, namely,  $t_L\gg t_d$  we show in Sect. 5 that alignment due to photodesorption may be efficient. We do not dwell upon all these interesting possibilities here, as believe, that the alignment of suprathermally rotating grains under the simultaneous action of several processes deserves a separate study.

Consider the alignment of grains subjected to Alfvénic perturbations. If, for the sake of simplicity, we approximate grains by thin discs the cross section will vary as

$$S_n = \pi r^2 |\sin \varphi \cos \psi| \tag{7}$$

where  $\varphi$  is the angle between the disc axis and magnetic field,  $\psi$  is an angle in the plane perpendicular to the magnetic field and |..| denote that we take the absolute value of the trigonometric functions. To account for the Larmour precession, we should perform averaging over  $\psi$ . Therefore,

$$\langle \cos^2 \varphi \rangle = C \int_0^{2\pi} \frac{d\psi}{|\cos \psi|} \int_0^{\pi} \cos^2 \varphi d\varphi \tag{8}$$

where the normalization constant C is

$$C^{-1} = \pi \int_0^{2\pi} \frac{d\psi}{|\cos\psi|}.$$
 (9)

In short, it is easy to see that  $\langle \cos^2 \varphi \rangle = 0.5$  and the Rayleigh reduction factor (Greenberg, 1968), is equal to 0.25. Grain long axis tends to be perpendicular to magnetic field, but the alignment is not perfect (compare Paper I).

In another important case, when flakes stream along magnetic field lines, similar computations provide  $\sigma=-0.5$ , which corresponds to the perfect alignment with grain long axis along magnetic field. More efficient alignment for streaming along magnetic field as compared with Alfvénic perturbations is a consequence of the fact, that in the former case the Larmour precession does not change the grain – gas cross section.

It easy to see, that this type of alignment is efficient for flakes, as the cross section difference averaged over the period of rotation is maximal for such grains. Contrary to this, the difference in cross sections is not large for prolate grains. For instance, for needles the ratio of the maximal to minimal averaged cross sections is just  $\pi/2$  and the  $\sigma$  for the most favorable conditions (a flow parallel to the magnetic field lines) is about 0.07. Therefore the alignment of prolate grains is marginal due to the mechanism.

It was implicitly assumed above that the angular momentum associated with gaseous bombardment is not important during a crossover. It is possible to show that, this is true unless grain drift velocity is comparable with velocity of  $\rm H_2$  molecules and/or accommodation coefficient is substantially different from unity and/or atomic hydrogen is largely converted into molecular form. A detailed discussion of the effects of gaseous bombardment is given in Lazarian (1995c).

# 4 PURCELL ALIGNMENT

We will call paramagnetic alignment of suprathermally rotating grains the Purcell alignment to distinguish it from the Davis-Greenstein mechanism acting on thermally rotating grains. Various aspects of the Purcell alignment were addressed in Paper II. Here we extend one aspect of the aforementioned analysis, namely, the one dealing with poisoning of active sites.

Back in Paper II it was established that a critical number of active sites exists. This number,  $\nu_{cr}$ , is the mean number of sites with chemically adsorbed H atoms, that a hydrogen atom arriving to the grain surface can visit before reacting at any of these sites. It is easy to see that, if the number of active sites is less than  $\nu_{cr}$ , there cannot be on average more than one active site, which is left empty since a recent H<sub>2</sub> formation. However, if the number of active sites  $\nu$  is greater than  $\nu_{cr}$ , the number of empty sites scales as  $\nu/\nu_{cr}$  for  $\nu_{cr} \gg 1$ . These empty sites are the primary targets of oxygen atoms hopping over grain surface and it was observed in Paper II that for  $\nu > \nu_{cr}$  poisoning increases. Therefore only the case of  $\nu < \nu_{cr}$  was discussed. Here we study the case of  $\nu > \nu_{cr}$ . Similarly to Paper II we assume that oxygen is being immobilized on hydrogenation (Leitch-Devlin & Williams 1984, Williams, private communication).

If  $\nu/\nu_{cr}$  is the expected number of empty active sites, the probability of an oxygen atom to fill any of them as a result of an individual hop is  $\nu/(\nu_{cr}N_{ph})$ , where  $N_{ph}$  is the number of sites of physical adsorption. Therefore the probability of an empty site not to be filled in one hop of an oxygen atom is  $(1 - \nu/(\nu_{cr}N_{ph}))$ ; the same probability for  $m_h$  hops is

$$\left(1 - \frac{\nu}{\nu_{cr} N_{ph}}\right)^{m_h} \approx \exp\left(-\frac{\nu}{\nu_{cr}} \frac{m_h}{N_{ph}}\right).$$
(10)

Therefore the characteristic time of poisoning of  $\nu/2$  active sites is  $^{\ddagger}$ 

$$t_p = \nu t_O \frac{1}{1 - \exp\left(-\frac{\nu}{\nu_{cr}} \frac{m_h}{N_{ph}}\right)},\tag{11}$$

<sup>&</sup>lt;sup>†</sup> We should bear in mind that Eq. (6) is an approximate one and it is checked in the range of  $0.1 < t_L/t_d < 10$  (Purcell 1979).

<sup>&</sup>lt;sup>‡</sup> We assume that not more than one oxygen atom hop over grain surface at any particular time. This may not be true for dense cores of molecular clouds, where the concentration of atomic hydrogen is low.

where  $t_O$  is the time of an oxygen atom arrival at grain surface. For  $\frac{\nu}{\nu_{cr}} \frac{m_h}{N_{ph}} \ll 1$  it is possible to expand the exponent in Eq (10)

$$t_p \approx \nu_{cr} t_O \frac{N_{ph}}{m_h} \left[ 1 + \frac{1}{2} \frac{m_h}{N_{ph}} \frac{\nu}{\nu_{cr}} - O\left(\frac{m_h^2}{N_{ph}^2} \frac{\nu^2}{\nu_{cr}^2}\right) \right].$$
 (12)

The number of hops  $m_h$  is the ratio of the time required to hydrogenate oxygen, which we denote  $t_{ch}$  to the time of an individual hop  $t_h \approx 10^{-12} \exp(E_h/(kT_s))$  s, where  $E_h$  is the energy of potential barrier and  $T_s$  is the grain temperature. When the number of active sites exceeds  $\nu_{cr}$  any hydrogen atom scans only the fraction  $\nu_{cr}/\nu$  of the entire surface before either reacting with another H atom at the active site or being trapped by an empty active site. The probability, that O atom adsorbed by the grain is present over this part of the surface is proportional to  $\nu_{cr}/\nu$ . Therefore the time hydrogenation of oxygen is of the order of the  $\nu/\nu_{cr}$  over the timescale of hydrogen arrival. Therefore

$$t_p \approx \nu_{cr} \frac{\nu_{cr}}{\nu} \frac{t_O}{t_H} t_h N_{ph} \left[ 1 + \frac{1}{2} \frac{\nu^2 t_H}{\nu_{cr}^2 t_h N_{ph}} - O\left(\frac{\nu^4 t_H^2}{\nu_{cr}^4 t_h^2 N_{ph}^2}\right) \right], (13)$$

where the ratio  $t_O/t_H = (\gamma_1 n_H v_O)/(n_O v_H)$ ;  $n_H \& v_H$  and  $n_O \& v_O$  are the densities & velocities of, respectively, hydrogen and oxygen. Note, that for thermal motions  $v_O/v_H$  is equal to 0.25.

If the ratio  $\eta = \nu/N_{ph}$  stays constant for different grains, it is evident from Eq.(13) that  $t_p$  at the first approximation is  $\approx 0.25 \frac{\nu_{cr}^2}{\eta \gamma_1} t_h \frac{n_H}{n_O}$ , i.e. it is independent of the number of active sites for  $\nu > \nu_{cr}$ . This is a new result, which was not foreseen in Paper II. This result means, for instance, that the estimates of  $t_p$  obtained there for  $\nu = \nu_{cr}$  are applicable to a wide range of grains with  $\nu > \nu_{cr}$ .

Poisoning of active sites is essential for the Purcell alignment. A parameter that enters this theory is the ratio of  $t_x$  given by Eq.(6) to the time scale of paramagnetic relaxation  $t_{mag}$  (see eq. (58) in Purcell 1979, also see Roberge et al 1993). To provide sufficient alignment this ratio should be greater than unity (see fig.2 in Purcell 1979). To obtain this for standard values of the ISM parameters  $\S$  one needs to assume long-lived spin-up, i.e.  $t_L \gg t_d$  (Spitzer & McGlynn 1979) and therefore  $t_x \sim t_L$ . It is easy to check that  $t_{mag}$  scales as  $l^2$ , where l is a grain size and therefore on its own paramagnetic alignment favors small grains (see Johnson 1982). For  $\nu > \nu_{cr}$  in the first approximation we have obtained that  $t_p$  scales as  $l^0$  (see Eq. (12)).

Note, that for  $\nu < \nu_{cr}$  our arguments above are not applicable. The corresponding study in Paper II showed, that in this case not more than one active site is expected to be empty and the time of poisoning is proportional to  $\nu t_O N_{ph}/m_h$  for  $m_h \ll N_{ph}$ . The number of hops for  $\nu < \nu_{cr}$  is the ratio of time scale of the arrival of a hydrogen atom  $t_H$  and the time scale of the hop of the oxygen atom  $t_h$ . Therefore both  $t_O$  and  $m_h$  scale as  $l^{-2}$ , while both  $N_{ph}$  and  $\nu$  scale as  $l^2$ . As a result the time of poisoning scales as  $l^4$ , which makes long-lived spin-up more probable for large grains.

In general, the life time of Purcell's rockets  $t_L$  is the minimal of the following time scales:  $t_p$  and the time scale of accreting one monolayer of refractory material. In diffuse clouds, as a rule, accreting of ice mantles is suppressed (see Tanaka et al 1990). It is also believed, that hydrogenated nitrogen and carbon within diffuse clouds do not form mantles either. As the abundance of heavier elements is negligible, it is natural to assume that in diffuse clouds  $t_L$  is controlled by poisoning of active sites.

Above we disregarded photodesorption. The characteristic time for this process  $t_{pd}$  scales as  $l^0$  for smooth grains. The situation  $t_{pd} \gg t_p$  corresponds to that studied in Paper II. If  $t_{pd} < t_p$ , photodesorption removes molecules blocking the access to active sites quicker that these sites are being poisoned. Thus a long-lived spin-up is called into being.

As a result the following qualitative picture emerges. For small grains poisoning dominates, i.e.  $t_{pd} > t_p$ , and therefore the spin-up is short-lived. The time of poisoning for  $\nu < \nu_{cr}$  grows with the size as  $t^4$  and for some size becomes equal to  $t_{ph}$ . Starting from this size we deal with long-lived spin-up;  $t_L$  grows with the size until  $\nu = \nu_{cr}$ . After the critical number of active sites is exceeded,  $t_L$  is stabilized at the attained level. In other words, marginal alignment is expected for small grains and good alignment for large grains; this corresponds to observations (see Kim & Martin 1994, Kim & Martin 1995).

Using both results obtained above and in Paper II we may attempt to write equations for the dinamics of the number of active sites. Indeed, while photodesprption, cosmic ray bombardment etc. create (or recover) active sites, poisoning removes them. The rate of active site creation per unit area A may be assumed constant, while the rate of poisoning is different for  $\nu < \nu_{cr}$  and  $\nu > \nu_{cr}$ .

If  $\nu < \nu_{cr}$  the results obtained in Paper II indicate, that the rate of poisoning can be approximated by  $CN_{ph}^{-1}$ , where  $C = 10^{12} \exp(-E_h/kT_s) \text{ s}^{-1}$ , while this rate is of the order of  $CN_{ph}^{-1}\nu^2\nu_{cr}^{-2}$  if  $\nu > \nu_{cr}$ . Therefore for  $\nu < \nu_{cr}$  the number of the active sites changes as

$$\frac{\mathrm{d}\nu}{\mathrm{d}t} = A - C \frac{1}{N_{nh}},\tag{14}$$

while for  $\nu > \nu_{cr}$  the following equation is valid:

$$\frac{\mathrm{d}\nu}{\mathrm{d}t} = A - C \frac{1}{N_{nh}} \frac{\nu^2}{\nu_{cr}^2}.\tag{15}$$

Evidentely, Eq. (14) envisages a linear change of the number of active sites. If the rate of desorption is greater than poisoning, the number of active sites will increase linearly with time, unless all the possible active sites are invoked over grain surface, provided, that this number is less than  $\nu_{cr}$ ) or alternatively the number of active sites is reached  $\nu_{cr}$ . In the opposite case when the rate of desorption is less than the rate of poisoning the number of active sites decreases with time untill all the active sites disappear. If  $\nu > \nu_{cr}$  the solution of the Eq. (15) is as follows:

$$\nu = \nu_{cr} \sqrt{\frac{AN_{ph}}{C}} \frac{1 + B \exp(-\frac{2}{\nu_{cr}} \sqrt{\frac{AC}{N_{ph}}} t)}{1 - B \exp(-\frac{2}{\nu_{cr}}, \sqrt{\frac{AC}{N_{ph}}} t)}.$$
 (16)

where B is related to the number of active sites  $\nu_{in}$  at t=0 in the following way:

<sup>§</sup> It is argued in Paper II that these standard values may be misleading for particular regions of diffuse clouds, but we avoid discussing this issue here.

$$B = \frac{\nu_{in} - \sqrt{\frac{A}{C}}}{\nu_{in} + \sqrt{\frac{A}{C}}}.$$
(17)

Eq. (16) testifies, that the number of active sites tend to stabilize at the level  $\nu_{cr}\sqrt{AN_{ph}/C}$ . Therefore for A a bit larger than  $C/N_{ph}$ , the number of active sites is expected to be of the order  $\nu_{cr}$  in correspondence with a qualitative conclusion reached in Paper II.

Unfortunately, in our ignorance of many parameters involved, it is extremely difficult to quantify this otherwise luring picture. First of all, we have rather uncertain knowledge of the density of active sites as well as of other parameters of grain surface. Then, photodesorption presents another problem, as the rates obtained in some laboratory experiments (see Bourdon, Prince & Duley 1982) are very low. We are not sure either whether the photodesorption is driven by UV quanta only or also by 3  $\mu$ m radiation as it is claimed in Williams et al (1992).

In view of this ambiguities, we need to treat the picture above as a conjecture only. We believe, that further research in the field will test this conjecture.

An interesting feature of Eq (13) that it shows that  $t_p$  is proportional to the number of sites of physical adsorption. Therefore fractal grains with large surface area should correspond to larger  $N_{ph}$ . The alignment of fractal grains was studied in Lazarian (1995d), where the excess of the physical area for such grains over that for smooth grains was invoked in order to improve the efficiency of alignment. This study indicated a possibility of a substantial improvement of alignment, provided that molecules blocking the access to active sites had sufficient mobility. This assumption seems to be a shortcoming of the latter study. However, it is possible to show that the dependences for alignment measure on the fractal dimension obtained in Lazarian (1995d) are valid without this assumption just as the result of the dependence of  $t_p$  on  $N_{ph}$ . Another worry in Lazarian (1995d) was, that for fractal grains the majority of H<sub>2</sub> formation events may take place within narrow pores, and this may suppress suprathermal rotation. Our arguments above show, that the sites within grain pores are likely to be poisoned and therefore H<sub>2</sub> formation should take place mainly over open surfaces of grains, which are kept clean e.g. due to photodesorption. At the same time, surfaces within pores provide oxygen with more space for its random walk hopping.

To summarize, we have shown, that the Purcell (1979) mechanism analogously to the Mathis (1986) one favors large grains. To tell these two mechanisms it is advantageous to study dependences of degree of alignment on grain temperatures. Our discussion above indicates, that  $t_p$  is proportional to  $t_h$ , which varies exponentially with temperature. Therefore the Purcell alignment, unlike the Mathis one should be very sensitive to changes of grain temperature.

Above we assumed that initially the concentration of active sites over grain surface is high. Although this corresponds to the modern picture of grain chemistry (see Tielens & Allamandola 1987, Buch & Zhang 1991), an alternative approach to the problem is also possible. Indeed, if the surface density of active sites may be less than  $10^{-5}$  cm<sup>2</sup> and than only grains larger than  $10^{-5}$  cm are likely to have at

least one active site (Lazarian 1994b).  $\P$  This idea requires further study, but here we would like to point out, that the case of high and low density of active sites can be distinguished by temperature dependence. It is easy to see, that if the density of active sites is low, while nascent  $H_2O$  molecules are ejected on formation, the temperature dependence of the Purcell alignment is suppressed.

# 5 OTHER POSSIBILITIES OF ALIGNMENT

Alignment of helical grains. Grains studied above were symmetric. However, real grains may have helicity. In fact, grains in Purcell (1975, 1979), that rotate suprathermally due to variations of the accommodation coefficient or photoelectric emission coefficient are helical. What was omitted in the above study is that the two aforementioned effects can produce alignment even without paramagnetic relaxation. For instance, radiation is, as a rule, anisotropic and this may influence the rotation caused by photoelectric emission.

There is a substantial difference when a helical grain is subjected to a isotropic bombardment of atoms or photons and when it is subjected to a flux. In the former case, there is no difference between  $\rm H_2$  formation and other causes of suprathermal rotation; with high degree of accuracy it is possible to assume, that the regular torque acts only along the axis of major inertia (see Spitzer & McGlynn 1979). If, however, a helical grain is subjected to a radiative or corpuscular flux, the component of torque perpendicular to the axis of major inertia can cause precession, which may significantly alter the alignment.

An interesting example of helical grains was discussed in Dolginov & Mytrophanov (1976). There, grains subjected to regular torques due to the difference in scattering of left-and right- circular polarized photons were considered. It was found, that if grains, either due to their chemical composition or due to their shape, have different cross-sections for left- and right-hand polarized quanta (see Dolginov & Silantev 1976) their scattering of unpolarized light results in the spin-up. The efficiency of this process is maximal for wavelengths  $\sim l$ . For twisted prolate grains, increments of grain angular momentum can be shown (Dolginov & Mytrophanov 1976) to be of the order of  $0.25\Phi_p\hbar l^2(n_r-1)^4$ , where  $\Phi_p$  is the flux of photons and  $n_r$  is the refraction coefficient ( $\sim 1.3$ ). Then the characteristic angular velocity is

$$\Omega \approx \frac{1}{8} \frac{\Phi_p (n_r - 1)^4 \hbar}{n m_\sigma v_o l^2},\tag{18}$$

which is of the order  $10^7 \, \mathrm{s^{-1}}$  for the typical concentration of photons in the ISM  $\sim 3 \cdot 10^9 \, \mathrm{cm^{-2} \, s^{-1}}$  and may become much higher in the vicinity of bright sources. For optimal shape suggested in Dolginov & Mytrophanov (1976) the scattering efficiency is sufficient to account for the alignment over vast regions, but one may expect the grains to have relatively small deviations towards the optimal form. Such grains are believed to be a natural product of evolution (Mathis 1990). However, numerical studies of the interaction of irregular grains with radiation by Bruce Draine (private

 $<sup>\</sup>P$  I suggested this possibility, but did not treat it seriously untill it got support from John Mathis.

communication) showed, that grains that do not resemble helicies can exibit high efficiency of spin-up due to scattering of radiation. These studies can shed the light on the problem, whether grain spin-up arising from light scattering is an exeption or a rule. Note, that such a spin-up is expected to be long-lived one. Indeed, it is not the surface, but grain volume, that should be altered substantially to cause a crossover event. Such a change is expected to take place over timescale much longer as compared with the time of gaseous damping, which means that the spin-up should be long-lived. For such a spin-up the alignment is nearly perfect just due to paramagnetic relaxation.

However, helical grains can be aligned mechanically on the timescale much shorter than the one relevant to the paramagnetic alignment. Mechanical alignment of helical grains is a complex problem and we are going to subject this issue to scrutiny in our next paper. Here we just refer to the study in Dolginov & Mytrophanov (1976) where it was shown, that grains asymptotically tend to align perfectly with their helicity axes along the direction of magnetic field, if the time of precession is much less than that of alignment, and along the flux direction, if the opposite is true. In their paper Dolginov & Mytrophanov considered a tilted oblate grain which helicity axis coincided with the major inertia axis and a tilted prolate grain where the two axis were perpendicular. The conclusion reached in Dolginov & Mytrophanov (1976) was that the two species subjected to a flux should be aligned orthogonally. However, the above study omits the influence of internal relaxation. Due to this effect a prolate grain initially rotating about its axis of minimal inertia will in a short period of time turn to rotate about the axis of major inertia. In other words, long axis of prolate and oblate grains should be aligned in the same direction.

To obtain quantitative results applicable to the ISM and circumstellar regions one needs to estimate the relative importance of this particular type of suprathermal rotation. Estimates in Purcell (1979) show that, as a rule, angular velocity of rotation due to  $\rm H_2$  formation should dominate for the ISM. Therefore, it seems unlikely that alignment due to grain helicity is more important in diffuse clouds in comparison with the one discussed in Sect. 3. However, the alignment of helical grains may be essential in the vicinity of bright sources.

Alignment due to radiation fluxes. Above we discussed both mechanical and paramagnetic alignment of suprathermally rotating grains. One may wonder whether alignment can be caused by absorption of quanta. Indeed, due to absorption of an individual quantum a grain gains  $\hbar$ angular momentum. This physical process is invoked in Harwit (1970). However, it was shown later in Purcell & Spitzer (1971) that if a grain is being subjected to a radiation flux, the drift produced by the radiation pressure entails Gold alignment, which is far more efficient than the Harwit one. It is not difficult to show, that the ratio of squared increments of angular momentum for the Harwit process  $\langle (\triangle J_H^2) \rangle$ to the one for the Gold process  $\langle (\triangle J_G^2) \rangle$  is negligible even for rather special conditions of alignment discussed in Aitken et al (1985). Note, that in the aforementioned study the Gold alignment was neglected and therefore a conclusion, that Harwit mechanism is efficient was reached. We claim, that this inference can be true only, if the Gold alignment is suppressed. The latter happens, for instance, if charged grains are trapped by close loops of magnetic field and cannot be accelerated under radiation pressure. In any case, such an inefficient process as a Harwit one, is unlikely to influence the dynamics of suprathermally rotating grains.

This, however, does not mean, that radiation cannot influence alignment of suprathermally rotating grains in a way other than through differential scattering of circular polarized quanta. For instance, we may suggest a mechanism based on photodesorption. Indeed, if suprathermal rotation is due to H<sub>2</sub> formation, we may refer to the toy model discussed in Sect. 3, but use a radiation flux instead of gaseous one. If this radiation flux desorbs molecules blocking the access to active sites, the life time of Purcell's rockets and therefore  $t_L$  will be different for  $\perp$  and  $\parallel$  orientation of our grain. It is easy to see, that this alignment is most efficient if  $t_L \gg t_d$ . However, in some cases, e.g. for hot and small grains discussed in Purcell & Spitzer (1971), the radiation dumping may dominate the gaseous one. In this case the grain temperature should depend on the grain orientation and  $t_L \gg t_d$  is not required for efficient alignment. However, a detailed study of these processes is beyond the scope of our present paper.

Alignment due to grain magnetic moments. To make our discussion more complete, we need to mention the alignment due to grain magnetic moments. One of the causes of these moments can be charge (Martin 1971, Draine & Salpeter 1979, Draine & Sutin 1987) over rotating grains (Rowland effect). The torques that act on a rotating charged grain were studied in Davis & Greenstein (1951), along with their famous prediction of paramagnetic alignment. However, the influence of the ambient gas was omitted in their analysis, and thus the conclusion that the 'distribution must be completely independent of the field' was made. This was quoted in other sources and therefore may still cause confusion

Consider an isolated rotating charged grain in magnetic field. Its rotation creates a magnetic moment  $\mathcal{M} = \Sigma_i \mathbf{e}(2c)^{-1} a_i^2 \mathbf{J}(I)^{-1}$ , where  $a_i$  is the distance from an elementary charge over the grain surface to the axis of rotation. This causes grain precession in the magnetic field according to the Larmour equation

$$\frac{\mathrm{d}\mathbf{J}}{\mathrm{d}t} = \mathcal{M} \times \mathbf{B} = \omega_g \mathbf{J} \times \frac{\mathbf{B}}{|\mathbf{B}|}$$
(19)

where  $\omega_g = \sum \frac{\mathrm{ea}_i^2 B}{3cI}$ , which is quite close to the grain Larmour frequency  $\omega_L$ . In the course of this precession the angle between  $\mathcal{M}$  and  $\mathbf{B}$  does not change, i.e. the precession by itself cannot change the energy of the system. The calculations in Davis & Greenstein (1951) reflect this fact. However, the energy changes due to the interaction of grains with surrounding gas. Indeed, the impact in the direction of the Larmour precession arising from grain interaction with an atom results in the torque, that cause the precession around the axis which is perpendicular to the magnetic field. Eq. (19) shows that the angle between  $\mathcal{M}$  and  $\mathbf{B}$  increases. If the impact is directed against the direction the Larmour precession, this angle decreases. The collisions of the first type

Note, that in reality we assume a uniform distributions of

disalign  $\mathcal{M}$  and  $\mathbf{B}$ , while the collisions of the second type align the two vectors. The alignment effect prevails as the impacts against precession are stronger than those in the direction of precession.

In our arguments above we used the fact, that the Larmour precession influences the direction, but not the magnitude of the vector **J**. Therefore the magnitude of  $\mathcal{M}$  (i.e.  $|\mathcal{M}|$ ) is not altered by the Larmour precession. In fact, in terms of grain interaction with magnetic field, the grain behaves as a magnetic dipole and the alignment due to the Rowland effect is similar to the alignment of magnetic dipoles. Such an alignment is not complete due to random torques acting upon grains.\*\* These random torques determine the effective temperature T and this temperature influences the equilibrium distribution of  $\mathcal{M}$ . If the suprathermal rotation is caused by the variations of the accommodation coefficient (see Purcell 1979), this temperature will be the mean of the grain and gas temperatures, provided that gasgrain collisions are inelastic. In the case of the suprathermal rotation caused by H<sub>2</sub> formation, T will be of the order of  $E_{H2}/k$ , provided that every hydrogen atom that hits grain surface leaves it as a part of H<sub>2</sub> molecule.

Indeed, if the spin-up is very long, then grains should behave as magnetic moments whose motion is disturbed by stochastic torques due to  $\rm H_2$  formation. These magnetic moments are peculiar in a sense, that the randomization of their precession requires time much greater than usual damping time. However, if the life time of Purcell's rockets exceeds this time, the treatment in mu228rv2 should be applicable.

In the extreme case of the short spin-up, when all torques are essentially stochastic one may introduce the averaged magnetic moment and study precession of this moment in the magnetic field. Our arguments should be applicable and the damping of the precession should occur over the timescale of the order of rotational damping time.

The equilibrium distribution of grain axes of major inertia in magnetic field B is proportional to  $\exp(-\mathcal{E}/(kT))$ , where  $\mathcal{E} = -\mathcal{M}\mathbf{B}$ . It is easy to see that

$$\frac{\mathcal{E}}{kT} \approx \frac{e}{2c} l^2 \frac{\omega_T B}{kT} \sim \frac{\omega_L}{\omega_T}$$
 (20)

for a thermally rotating grain and  $\mathcal{E}(kT)^{-1} \approx \omega_L \omega_r \omega_T^{-2}$  for a suprathermally rotating grain,  $\omega_T$  is the frequency of rotation corresponding to the temperature T,  $\omega_r$  is the frequency of the suprathermal rotation and  $\omega_L$  is the Larmour frequency.

In fact, grain alignment due to the Rowland effect is in no way different from the alignment of ferromagnetic grains with high permanent magnetization discussed in Spitzer & Tukey (1951). The difference is of quantitative nature; ferromagnetic grains have much larger magnetic moments and therefore much more susceptible for such an alignment. However, even with ferromagnetic grains the alignment was

atomic impacts and subdivide the impacts as having component either in the direction of the precession or opposite to it.

shown to be not efficient for diffuse clouds  $^{\ddagger \ddagger}$  (Spitzer & Tukey 1951). Therefore alignment due to the Rowland effect is negligible for the majority of the foreseeable cases. This a fortiori true, as paramagnetic grains obtain much larger magnetic moments through the Barnett, rather than through Rowland effect. Assuming that  $\omega_T \approx 10^5 \text{ s}^{-1}$ ,  $B \approx 3 \times 10^{-6} \text{ G}$ ,  $\omega_r \approx 10^4 \omega_T$ , we still fall short by approximately six orders of magnitude to produce any measurable alignment due to this effect.

To summarize, magnetic moments irrespectively of their nature (the Rowland effect, the Barnett effect, permanent magnetization) do produce alignment, but this alignment is negligible for suprathermally rotating grains in diffuse clouds.

#### 6 CONCLUSIONS

Several mechanisms of alignment of suprathermally rotating grains were discussed and it was shown that

- I. Paramagnetic alignment stays the strongest candidate to account for grain alignment over vast regions of the diffuse clouds. Its modification suggested in Purcell (1979) depends on subtle processes over grain surfaces and this provides an opportunity to test it.
- II. Alignment of grains due to the cross section effect that was introduced in this paper can also be important for the diffuse ISM. This mechanism, similar to the paramagnetic one, tends to align long grain axis perpendicular to magnetic field lines, provided that the grain drift is caused by Alfvénic perturbations.
- III. Radiation can drive alignment in the vicinity of bright sources even in the absence of supersonic drift. Such an alignment is more likely to arise from differential photodesorption, although in some particular cases anisotropic radiation field can also provide the alignment of "helical" grains. Therefore additional care is required in interpreting the corresponding polarimetric data.
- IV. Magnetic moments of grains both arising from the Barnett effect and due to their charge produce alignment, but the expected degree of alignment is negligible.

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 $^{\ddagger\ddagger}$  It is possible to show that Spitzer & Tukey alignment may not be negligible in dark clouds, where both grain and gas temperatures are low, while magnetic fields  $> 10^{-4}$  are commonplace. However, such grains are not expected to rotate suprathermally and thus we do not discuss them there.

<sup>\*\*</sup> Thermal fluctuations within grain material can randomize alignment as well, but the influence of such fluctuations for suprathermally rotating grains is negligible.

<sup>&</sup>lt;sup>††</sup> Note, that we are speaking about averaged  $J^2$  components of the torque.

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